ANALYTICAL DESCRIPTION OF FREQUENCIES, DIPOLE STRENGTHS AND ROTATIONAL STRENGTHS FOR FUNDAMENTAL AND OVERTONE CH-STRETCHING TRANSITIONS

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The normal mode to local mode transition has been described in the past by basic arguments centered on symmetry and on perturbative-type numerical quantum mechanical calculations [ab]. In this work we investigate the absorption and Vibrational Circular Dichroism (VCD) spectra for a two degrees of freedom model of an HCCH chiral fragment endowed with C_2-symmetry, for the fundamental (Δv=1) and first two overtone regions Δv=2,3). We include electrical anharmonicity [c] in addition to mechanical anharmonicity, and deal with them in the framework of the Van Vleck contact transformation theory [de]. By making use of an algebraic manipulator (Maple) we are able to derive useful analytical expressions for frequencies, dipole strengths and rotational strengths for Δv=1,2,3.

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